

Substance Name	CASRN	In Vitro Concentration Tested	In Vitro Physical Form Tested	Purity (%)	Solubility ¹	pH	S-Score ²	S-Score Classification	Overall S-Score Classification	Reference
Ammonium nitrate	6484-52-2	100%	Solid	>99.9	water soluble		18.00	Severe	Severe	Balls et al. (1995)
Ammonium nitrate	6484-52-2	100%	Solid	>99.9	water soluble		12.00	Moderate		Balls et al. (1995)
L-Aspartic acid	70-47-3	100%	Solid	100	water soluble		1.00	Nonirritant	Nonirritant	Balls et al. (1995)
L-Aspartic acid	70-47-3	100%	Solid	100	water soluble		2.00	Nonirritant		Balls et al. (1995)
L-Aspartic acid	70-47-3	100%	Solid	100	water soluble		6.00	Moderate		Balls et al. (1995)
Benzoyl-L-tartaric acid	2743-38-6	100%	Solid	98	water insoluble		0.00	Nonirritant	Nonirritant	Balls et al. (1995)
Benzoyl-L-tartaric acid	2743-38-6	100%	Solid	98	water insoluble		4.00	Nonirritant		Balls et al. (1995)
Captan 90 concentrate	133-06-2	100%	Solid	90	water soluble		0.00	Nonirritant	Nonirritant	Balls et al. (1995)
Captan 90 concentrate	133-06-2	100%	Solid	90	water soluble		0.00	Nonirritant		Balls et al. (1995)
Captan 90 concentrate	133-06-2	100%	Solid	90	water soluble		6.00	Moderate		Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	100%	Solid	95	water insoluble		0.00	Nonirritant	Moderate	Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	100%	Solid	95	water insoluble		6.00	Moderate		Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	100%	Solid	95	water insoluble		6.00	Moderate		Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	100%	Solid	95	water insoluble		4.00	Nonirritant		Balls et al. (1995)
Chlorhexidine	55-56-1	100%	Solid		water insoluble		3.00	Nonirritant	Moderate	Balls et al. (1995)
Chlorhexidine	55-56-1	100%	Solid		water insoluble		6.00	Moderate		Balls et al. (1995)
Chlorhexidine	55-56-1	100%	Solid		water insoluble		11.00	Moderate		Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	100%	Solid	99.5	water insoluble		0.00	Nonirritant	Severe	Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	100%	Solid	99.5	water insoluble		18.00	Severe		Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	100%	Solid	99.5	water insoluble		0.00	Nonirritant		Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	100%	Solid	99.5	water insoluble		15.00	Severe		Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	100%	Solid	99.5	water insoluble		18.00	Severe	Severe	Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	100%	Solid	99.5	water insoluble		18.00	Severe		Balls et al. (1995)
Fomesafen	72128-02-0	100%	Solid	97.5	water soluble		0.00	Nonirritant	Moderate	Balls et al. (1995)
Fomesafen	72128-02-0	100%	Solid	97.5	water soluble		9.00	Moderate		Balls et al. (1995)
Fomesafen	72128-02-0	100%	Solid	97.5	water soluble		6.00	Moderate		Balls et al. (1995)
Fomesafen	72128-02-0	100%	Solid	97.5	water soluble		6.00	Moderate		Balls et al. (1995)
Imidazole	288-32-4	100%	Solid	99	water soluble		18.00	Severe	Severe	Balls et al. (1995)
Imidazole	288-32-4	100%	Solid	99	water soluble		18.00	Severe		Balls et al. (1995)
Maneb	12427-38-2	100%	Solid	ca. 90	water soluble		0.00	Nonirritant	Nonirritant	Balls et al. (1995)

Substance Name	CASRN	In Vitro Concentration Tested	In Vitro Physical Form Tested	Purity (%)	Solubility ¹	pH	S-Score ²	S-Score Classification	Overall S-Score Classification	Reference
1-Naphthalene acetic acid, Na salt	61-31-4	100%	Solid	99	water soluble		18.00	Severe	Severe	Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	100%	Solid	99	water soluble		18.00	Severe		Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	100%	Solid	96	water insoluble		6.00	Moderate	Moderate	Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	100%	Solid	96	water insoluble		13.00	Moderate		Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	100%	Solid	96	water insoluble		0.00	Nonirritant		Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	100%	Solid	96	water insoluble		4.00	Nonirritant		Balls et al. (1995)
Potassium cyanate	590-28-3	100%	Solid	97	water soluble		18.00	Severe	Severe	Balls et al. (1995)
Promethazine HCl	58-33-3	100%	Solid	98	water soluble		18.00	Severe	Severe	Balls et al. (1995)
Promethazine HCl	58-33-3	100%	Solid	98	water soluble		18.00	Severe		Balls et al. (1995)
Quinacrine	69-05-6	100%	Solid		water soluble		0.00	Nonirritant	Nonirritant	Balls et al. (1995)
Quinacrine	69-05-6	100%	Solid		water soluble		4.00	Nonirritant		Balls et al. (1995)
Quinacrine	69-05-6	100%	Solid		water soluble		3.00	Nonirritant		Balls et al. (1995)
Sodium oxalate	62-76-0	100%	Solid	>99	water soluble		0.00	Nonirritant	Moderate	Balls et al. (1995)
Sodium oxalate	62-76-0	100%	Solid	>99	water soluble		12.00	Moderate		Balls et al. (1995)
Sodium oxalate	62-76-0	100%	Solid	>99	water soluble		11.00	Moderate		Balls et al. (1995)
Sodium oxalate	62-76-0	100%	Solid	>99	water soluble		9.00	Moderate		Balls et al. (1995)
Sodium perborate	10486-00-7	100%	Solid	98.6	water soluble		0.00	Nonirritant	Nonirritant	Balls et al. (1995)
Sodium perborate	10486-00-7	100%	Solid	98.6	water soluble		0.00	Nonirritant		Balls et al. (1995)
Sodium perborate	10486-00-7	100%	Solid	98.6	water soluble		7.00	Moderate		Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	100%	Solid	97	water insoluble		0.00	Nonirritant	Nonirritant	Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	100%	Solid	97	water insoluble		0.00	Nonirritant		Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	100%	Solid	97	water insoluble		6.00	Moderate		Balls et al. (1995)
Thiourea	62-56-6	100%	Solid	>99	water soluble		18.00	Severe	Severe	Balls et al. (1995)
Thiourea	62-56-6	100%	Solid	>99	water soluble		13.00	Moderate		Balls et al. (1995)

Abbreviation: CASRN = Chemical Abstract Service Registry Number, HCl = Hydrochloric acid.

¹ Solubility obtained from literature sources, where available expressed as g/mL

² S-Score represents irritation scores that were calculated using the method described in Balls et al. (1995)